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# MODTRAN5: A Reformulated Atmospheric Band Model with Auxiliary Species and Practical Multiple Scattering Options

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## ABSTRACT

The MODTRAN5 radiation transport (RT) model is a major advancement over earlier versions of the MODTRAN atmospheric transmittance and radiance model. New model features include (1) finer spectral resolution via the Spectrally Enhanced Resolution MODTRAN (SERTRAN) molecular band model, (2) a fully coupled treatment of auxiliary molecular species, and (3) a rapid and high fidelity multiple scattering (MS) option. The finer spectral resolution improves model accuracy especially in the mid- and long-wave infrared; the auxiliary species will permit the addition of any or the entire suite of HITRAN species, along with default and user-defined profile specification; and the MS option makes feasible the calculation of Vis-NIR (Near InfraRed) databases that include high-fidelity scattered radiances.

**Keywords:** MODTRAN, remote sensing, hyperspectral, imaging, band model, infrared, radiative transfer, molecular transmittance

## 1. INTRODUCTION

MODTRAN<sup>1,2</sup> has served as the U.S. Air Force (USAF) standard moderate spectral resolution radiative transport model for wavelengths extending from the thermal InfraRed (IR) through the visible and into the ultraviolet (0.2 to 10,000.0  $\mu\text{m}$ ). The MODTRAN 1  $\text{cm}^{-1}$  statistical band model was developed collaboratively by Spectral Sciences, Inc. and the USAF Research Laboratory, and it provides a fast alternative (100-fold increase in speed) to the USAF first principles and more accurate line-by-line (LBL) radiative transport models, FASCOD<sup>3</sup> and FASCOD for the Environment, FASE<sup>4</sup>. Comparisons between MODTRAN and FASE spectral transmittances and radiances show agreement to within a few percent or better in the thermal IR. MODTRAN4 includes flux and atmosphere-scattered solar calculations, essential components in analysis of near-IR and visible spectral region data that are not readily generated by LBL models.

MODTRAN4 and its predecessors have been used extensively over the last quarter century in the design and analysis of broadband, multiband, and short-wave IR/Visible hyperspectral imaging sensors. However, conventional interferometers and many state-of-the-art and next-generation hyper- and ultra-spectral imaging sensors working in the long- and mid-wave IR will operate at finer spectral resolution than MODTRAN4 provides. These sensors will also produce increased data quality, quantity and utility. This has served as a primary impetus for development of MODTRAN5. The long-wave requirement for finer spectral resolution led to the reformulation of the MODTRAN band model equivalent width and line tail absorption algorithms. The result of that work is the 0.1  $\text{cm}^{-1}$  SERTRAN (Spectrally Enhanced Resolution MODTRAN) molecular band model. The finer spectral resolution model provides high quality fine resolution predictions. Development of SERTRAN has also led to improved coarser resolution statistical band models by providing a source for tuning the coarse spectral resolution databases and by refining the transmittance algorithms within MODTRAN.

The introduction of the auxiliary species option enables MODTRAN users to simulate the impact of trace molecular gases. User input of both profile and optical data is required. Auxiliary database files for all the HITRAN molecular species not already included in MODTRAN are being generated. In addition, the default vertical profiles for these HITRAN-specific gases will be made available. It is anticipated that a user-defined option for other gases and their profiles will eventually come on line.

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A new multiple scattering option automatically performs DISORT<sup>5</sup> multiple scattering calculations at a few fixed spectral points and then spectrally scales fast ISAACS<sup>6</sup> 2-stream results. In the visible and NIR transparent window regions, where multiple scattering is the dominant radiation source, the scaling dramatically improves the accuracy of predicted radiances. These MODTRAN5 advances are described in the following sections.

## 2. THE SERTRAN BAND MODEL

Narrowing the band model spectral resolution changes the fundamental character of the band model. The average half-width of molecular transitions near sea-level is of order  $0.07 \text{ cm}^{-1}$ , which is comparable to the SERTRAN spectral bin width. As illustrated in Figure 1, the  $1.0 \text{ cm}^{-1}$  statistical band model calculates the absorption of molecular lines whose line center regions lie almost entirely within the spectral bin. A much larger fraction of each molecular line falls outside of the spectral bin at the finer spectral resolution of SERTRAN. Reformulation of the molecular band model has therefore required improved treatment of both line center and line tail absorption. Line tail absorption must be modeled near line centers, and the finite-bin single-line equivalent width used to calculate line center absorption is not simply a small perturbation of the total single line equivalent width.

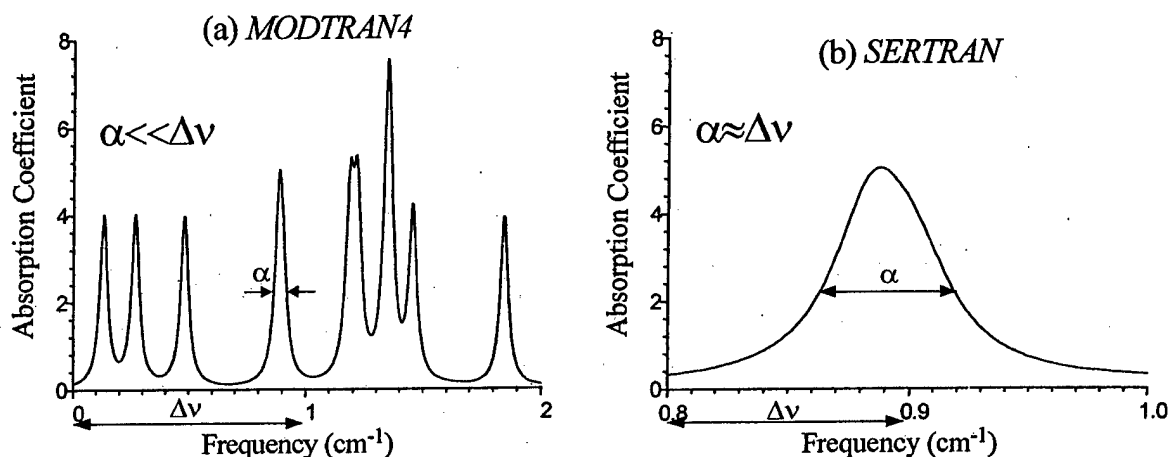


Figure 1. Molecular transition spectral absorption near the ground: (a) Spectral features within a MODTRAN  $1.0 \text{ cm}^{-1}$  bin; (b) Spectral features within a SERTRAN  $0.1 \text{ cm}^{-1}$  bin.

The band model line center absorption within a spectral bin is defined as the in-band absorption from all molecular transitions centered in that bin, Figure 2. LBL models calculate this in-band absorption by explicitly determining the spectral absorption of each molecular line on a fine spectral grid and then integrating the resulting spectra. In a band model approach, the in-band absorption is approximated by a statistical representation of the number of lines and their strength, location and overlap. Temperature-dependent band model data are computed from a molecular transition line atlas such as HITRAN<sup>7</sup>. These parameters define an effective single-line absorption strength for the interval and an effective number of lines.

The finite spectral bin single-line Voigt equivalent width is computed to determine the absorption of the effective average line. It is calculated as the difference between the total equivalent width and the absorption due to the line tails falling outside of the spectral band.

The line tail subtractions are performed for an off-centered line with the distance from spectral bin edge determined from the weak-line Lorentz limit. Offsetting the location of the effective line from the bin center lowers its in-band absorption, thereby producing a more representative result for a line randomly located in the bin.

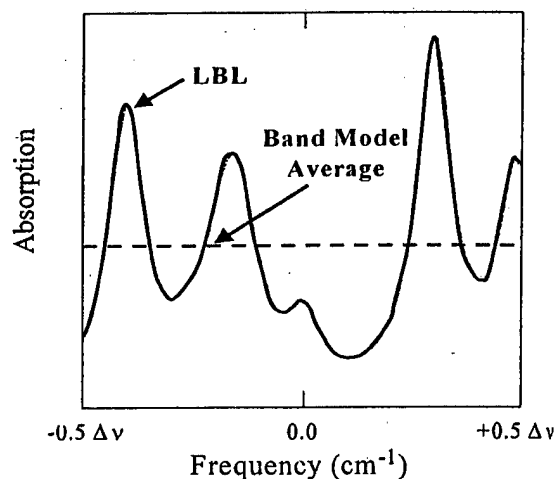


Figure 2. Comparison of Band Model and Line-By-Line Approaches. LBL models calculate high spectral resolution absorption (solid curve). Band models statistically determine the average integrated strength (dash line) based on line strength, line density, and line width parameters.

Line tails are not simply inversely proportional to square of the line center displacement (the MODTRAN4 assumption) when the spectral bin width ( $\Delta\nu$ ) is  $0.1 \text{ cm}^{-1}$  and the effective average line is positioned  $\Delta\nu/4$  from the bin edge. Neither are the line tails simply Lorentzian. In SERTRAN, the integrated Voigt line tails  $W_\Delta$  are computed from a newly derived exact expansion:

$$W_\Delta = Su \exp\left(-\frac{Su}{2} f_\Delta\right) \left[ \frac{V_0}{2} I_0\left(\frac{Su}{2} f_\Delta\right) + \sum_{n=1}^{\infty} V_n I_n\left(\frac{Su}{2} f_\Delta\right) \right] - \Delta [1 - \exp(-Su f_\Delta)] \quad (1)$$

Here,  $\Delta$  is the distance from line center,  $f_\Delta$  is the normalized Voigt line shape function,  $Su$  is the line strength and molecular column product,  $I_n$  are modified Bessel functions of integer order, and the  $V_n$  are Fourier expansion coefficients:

$$V_n = 2\nu P_n \Big|_{\nu=-\Delta}^{\nu=\Delta} + 2 \int_{-\Delta}^{\Delta} P_n d\nu \quad ; \quad P_n = \int_0^f \cos \left[ n \cos^{-1} \left( 1 - \frac{2f}{f_\Delta} \right) \right] df. \quad (2)$$

Details of the derivation of these expressions have been provided elsewhere<sup>8</sup>.

MODTRAN band model line tail absorption for a spectral bin is defined as the absorption from molecular transitions centered outside of the bin but no more than  $25 \text{ cm}^{-1}$  from band center. Contributions from beyond  $25 \text{ cm}^{-1}$  are modeled as continua. In MODTRAN5, the line tail spectral absorption is fit to temperature and pressure dependent Padé approximants. Five parameters,  $k_0, k_1, k_2, x_1$  and  $x_2$ , are used in the Padé fits:

$$\frac{k(\delta_\nu)}{P/P_0} = \frac{k_0 + k_1 \delta_\nu + k_2 \delta_\nu^2}{1 + x_1 \delta_\nu + x_2 \delta_\nu^2} \quad ; \quad \delta_\nu = \frac{\nu - \nu_{cen}}{\Delta\nu/2} \quad (3)$$

In this parameterization,  $\nu_{cen}$  is the central frequency of the spectral bin and the range of the normalized spectral variable  $\delta_\nu$  is from -1 to +1. Since the Lorentz line shape to leading order is proportional to pressure, the absorption coefficient over pressure  $P$  normalized to 1 atm ( $P_0$ ) is fit. This form for the tail contributions is exact in the limit of a single Lorentz tail. The five Padé parameters are determined from the summed line tail spectral absorption coefficients at  $\nu_{cen}$  and edges of the spectral band, the spectral frequency derivative of the absorption coefficient at  $\nu_{cen}$ , and the integral of the spectral absorption coefficient over the spectral band.

Figure 3 illustrates an example of a Padé spectral fit to line tail contributions. In this case, hundreds of molecular transitions contribute to the 305K and 1 atm pressure  $\text{H}_2\text{O}$  line tail absorption coefficient spectrum between 200.0 and 200.1  $\text{cm}^{-1}$ , the thick dashed curve. As is generally true, the spectral fit lies directly on top of the high-resolution spectrum.

The Padé parameter database is generated for 6 evenly spaced temperatures from 180 to 305K and for pressures of 1.0 and 0.1 atm. In MODTRAN, a parameter defines the number of monochromatic line tail absorption coefficient calculations per spectral bin; it is nominally set to 5. The line tail optical depth is modeled as varying linearly between spectral points for computing transmittances. The  $k/P$  interpolations are linear in temperature and in pressure squared.

MODTRAN5 spectral transmittances from  $\text{H}_2\text{O}$  absorption, nadir-viewing through the relatively wet Mid-Latitude Summer (MLS) model atmosphere, were compared to calculations from the Line-By-Line Radiation Transport Model<sup>9</sup> (LBLRTM). A common database of molecular line data, the HITRAN2k<sup>7, 10</sup> with 2001 updates, was used for these calculations. The spectral range extended from 0.88 to 1.22  $\mu\text{m}$ , spanning both the 0.94 and 1.38  $\mu\text{m}$   $\text{H}_2\text{O}$  bands. The results, illustrated for a small spectral subset in Figure 4, are typical. The overlay of MODTRAN5 and LBLRTM  $0.2 \text{ cm}^{-1}$  resolution spectra show excellent agreement. The more detailed residual curves (offset by 1.10 in Figure 4) show that deviations as large as 0.07 can arise. These substantial deviations are a result of the band model formulation, which requires that line centers be shifted by as much as  $0.025 \text{ cm}^{-1}$  from the edge of the  $0.1 \text{ cm}^{-1}$  spectral bands. The line center shifts in turn produce a shift of absorption between neighboring bands. As the results are further degraded, residual decrease and there is generally little or no biasing to too much or too little integrated absorption.

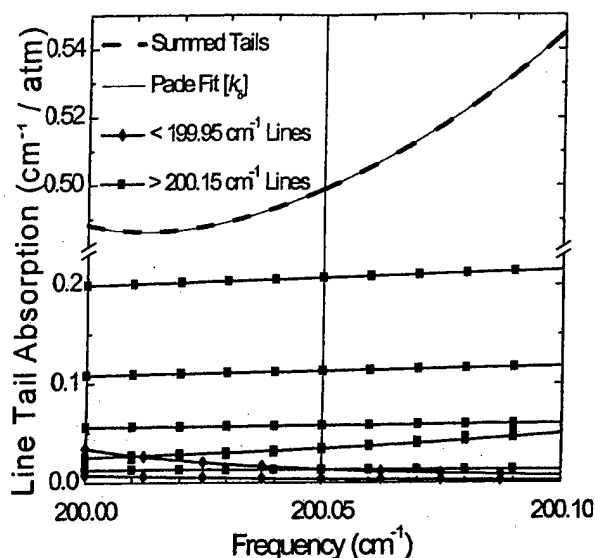


Figure 3. High Spectral Resolution Line Tail Absorption Curve (thick dash) and Padé Approximant Fit (thin line) for Lorentzian H<sub>2</sub>O Lines at 305K and 1atm Pressure. The spectral curves from largest contributors are also illustrated (lines with diamond for lower frequency transitions and lines with squares for higher frequency transitions).

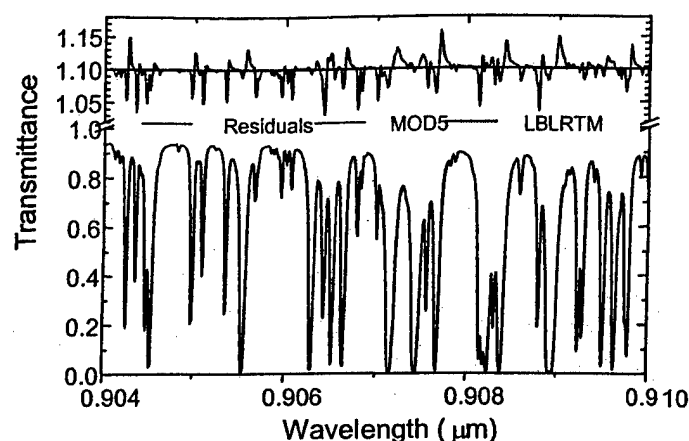


Figure 4. Intercomparison of 0.2 cm<sup>-1</sup> spectral transmittances for H<sub>2</sub>O between MODTRAN5 and LBLRTM. An offset by 1.1 has been added to the MODTRAN5 - LBLRTM residuals.

### 3. AUXILIARY SPECIES

In MODTRAN5, auxiliary species molecular densities can be defined via user-specified atmospheric vertical profiles or with the 'default' profiles currently provided with FASCODE/FASE. For each auxiliary species, MODTRAN5 accepts input of either MODTRAN-like molecular band model parameters or absorption cross-sections, similar to those already employed for the O<sub>3</sub> Chappuis bands (non-temperature dependent) or CFCs. The band model provides greater accuracy if optical depths are substantial, but absorption data is often more readily available for non-HITRAN species. Any of the NIST/EPA Gas Phase Infrared Database JCAMP-DX<sup>11</sup> (Joint Committee for Atomic and Molecular Physical Data "Data Exchange") measured absorption spectra as well as other gaseous database spectra can be introduced. However, because the actual database is the property of the measurement laboratories, MODTRAN5 will not be distributed with species spectral libraries, but only the conversion utility.

As the column amount of an auxiliary species increases, the growth of in-band optical depth slows and a band model is required to accurately compute absorption. As noted, band model data files are being generated for HITRAN species not already included in MODTRAN. Alternatively, band model data can be computed from either extensive compilations of transition frequencies, line strengths, lower state energies and collision broadened half-widths, or from absorption spectra as a function of molecular column density for a series of temperatures.

The mechanism for introducing auxiliary species is similar to that for MODTRAN standard atmospheric molecular species when user-defined profiles or radiosonde data are being entered. For each atmospheric level, the density of each species is input directly or is linked to a default profile. Unlike the standard molecules, the number of auxiliary species is read from the profile table header. This number is the total number of auxiliary species in the user's master list. The input to MODTRAN5 accepts a negative sign "-" prefix for any species name to indicate the species is to be excluded. This input format was instituted so that the input stream would not have to be completely reconfigured each time a species is to be added or removed. A star (\*) at the end of species name indicates band model rather than absorption coefficient data is to be read. The optical data for each species is stored in species-dependent auxiliary input files (SF6.BM for a SF<sub>6</sub> absorption coefficient file, SF6.CBM for a SF<sub>6</sub> line center band model data file, and SF6.TBM for a SF<sub>6</sub> line tail band model data file).

To illustrate the auxiliary species option, MODTRAN band model data files have been generated for HCl diatomic molecule, specifically, files HCl.CBM and HCl.TBM. A simple profile containing a surface layer of HCl was folded in the MODTRAN MLS model atmosphere by setting the HCl density to a constant value between 0.00 and 0.99km and having it ramp down to zero over the next 20 meters. MODTRAN nadir-viewing spectral transmittances and radiances were generated for HCl concentrations of 0.1, 1.0 and 10.0 ppm. For a Top-Of-Atmosphere sensor, HCl transmittance spectra are illustrated in Figure 5. On the left, the envelope of R and P branch transitions from the (0-1) vibrational transition are displayed. At 0.2  $\text{cm}^{-1}$  spectral resolution, the splitting of the  $\text{HCl}^{35}$  and  $\text{HCl}^{37}$  isotopes is resolved. This is illustrated for R2 and P3 transitions on the right in Figure 5.

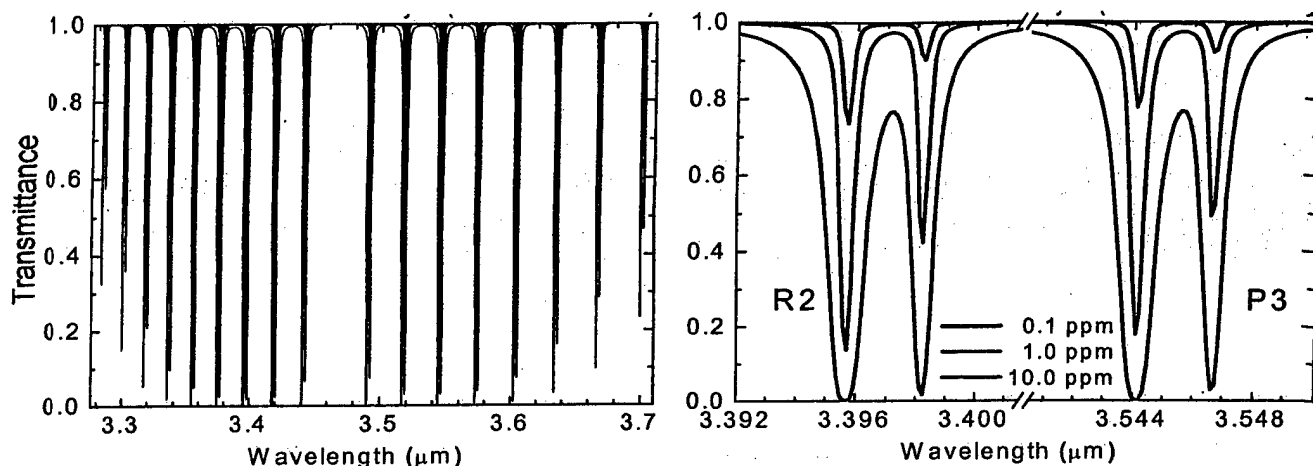


Figure 5. HCl Spectral Transmittances as Predicted by the MODTRAN5 using the Auxiliary Species Option

The transmittance spectrum of the R2 and P3 vibrational/rotational lines for the HCl fundamental arising from the HCl surface layer, when embedded in the MODTRAN MLS atmosphere and viewed from space, Figure 6, is considerably more complex than the spectrum of the isolated species because of spectral overlap with other molecular species. Both  $\text{CH}_4$  and  $\text{H}_2\text{O}$  have strong absorption lines in this spectral region. The profiles of these competing absorbers must be well characterized if HCl is to be correctly included in the simulation. There is, of course, a feedback between the temperature and the distribution of all gases in a radiative transfer calculation, whether modeled by a band model like MODTRAN or an LBL code. In Figure 6 the concentration of HCl increases, while the observed thermal emission increases. If, however, the surface temperature was not lowered, the effect of the added gas would have been to lessen the observed radiance. In effect, the HCl emission would be occurring at a lower atmospheric temperature than the background surface. Thus, the result from introducing auxiliary species (or altering the concentration and/or temperature of any of the extant species) is a complex function dependent on contrast between surface and gas temperatures.

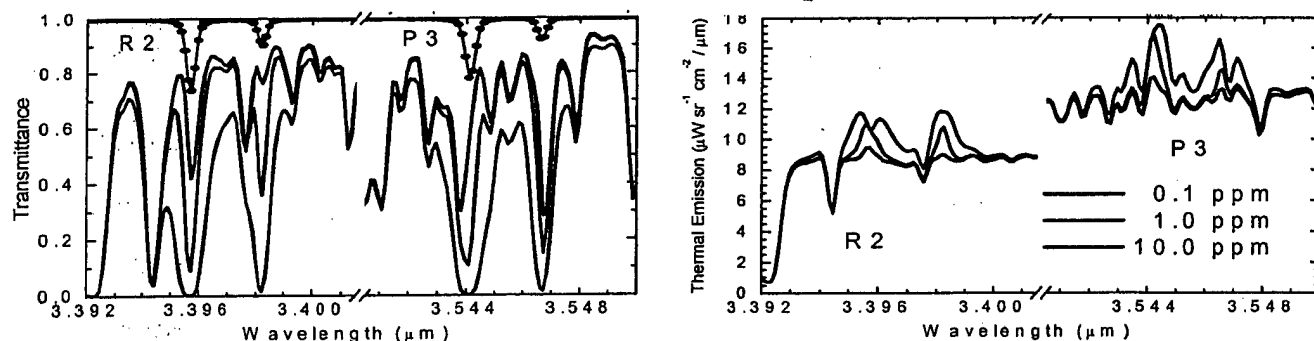


Figure 6. Spectral Transmittances and Thermal Emission as Predicted by the MODTRAN5 for Nadir-Viewing through a MLS atmosphere with a 1 km High HCl layer at the Surface. The blackbody ground temperature is 10K below the surface air temperature.

#### 4. RAPID ACCURATE MULTIPLE SCATTERING

Previous versions of MODTRAN provide two algorithms for computing the multiple scattering components of the total path radiance: an approximate ISAACS 2-stream method and the accurate but time-consuming multi-stream DISORT (DIScrete Ordinate Radiance Transfer) method. DISORT runs 100 to 1000 times slower than the 2-stream method. For MODTRAN5, an option has been developed to spectrally scale the 2-stream calculations using DISORT results at a small number of wavelengths. This scaling recovers almost full DISORT accuracy with less than a factor of two time penalty as compared to ISAACS.

The DISORT scaling works as follows. Twelve spectral wavelengths between 2.14 and 0.20  $\mu\text{m}$  have been selected lying outside of the stronger MODTRAN atmospheric molecular bands, Figure 7. These values are hardwired into MODTRAN5. Molecular bands are avoided because multiple scatter radiance contributions are less dominant in the presence of molecular absorption. As an automated preprocess within MODTRAN, DISORT and ISAACS multiple scattering path radiance calculations with the user-defined solar and path geometry are performed at the DISORT scaling wavelengths encompassing the input spectral range. Two spectral correction curves are generated from these calculations: one for the path scattered radiance (excluding single scatter solar) and the second for the downward diffuse flux at the ground. The corrections are defined as the ratio of the DISORT to ISAACS values and linearly interpolation between wavelengths. These spectral corrections are then applied to the ISAACS results computed at the band model spectral resolution.

Figure 8 illustrates the benefit of scaling. In this figure, spectral radiances are simulated for a nadir viewing from space and a  $40^\circ$  sun. The atmosphere was set to the MODTRAN mid-latitude summer with its relatively high water column. Aerosol loading was also relatively high with the surface meteorological range (visibility) input of 23-km and Navy Maritime aerosol type. The surface albedo is zero, so only the path multiple scattered radiance is scaled. The spectral radiance predictions in the visible spectral region (400-700nm) with ISAACS multiple scattering are  $\sim 10\%$  below the results with 8-stream DISORT. Introducing the scaling algorithm essentially eliminates these residuals. In the Near-IR, the overall performance of scaling is mixed. Outside of the strong molecular bands the scaling significantly improves the radiance results, but within molecular bands the scaling produces too much radiance. In these regions, best results are still obtained by performing the rigorous DISORT calculations.

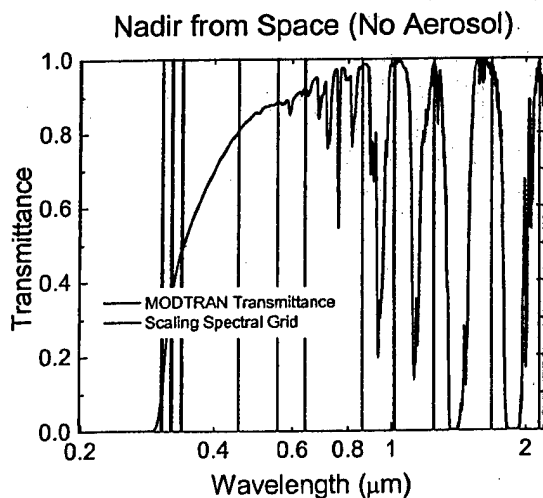


Figure 7. Spectral Grid for DISORT Scaling of ISAACS 2-Stream Multiple Scattering. Wavelengths are selected outside of strong atmospheric molecular bands.

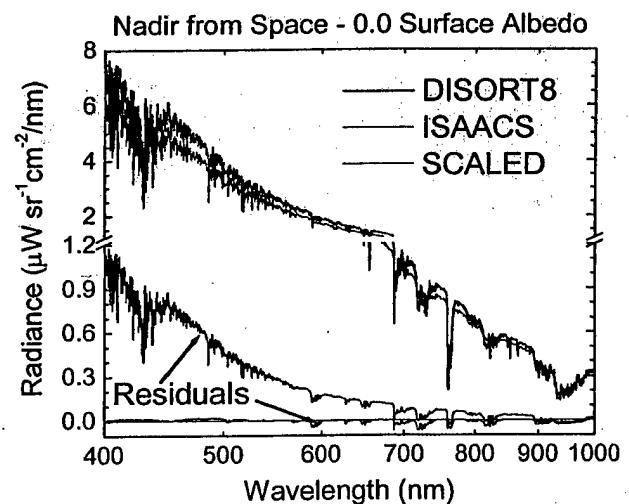


Figure 8. Results for DISORT Spectral Scaling of ISAACS Radiances with a Black Surface (Albedo = 0).

In a second example, the results of scaling are illustrated with a fully reflective ground surface, Figure 9. As expected, the spectral radiances are almost an order of magnitude higher than in Figure 8. The results of scaling remain good outside of molecular bands. Within these bands the residuals are substantial; for best results, DISORT should be used within these bands. The main benefit of scaling is in analysis and retrieval of aerosols. Traditionally, the spectral window regions have been exploited to extract aerosol loading and type. This analysis is greatly improved with accurate multiple scattering, which the DISORT scaling option provides.

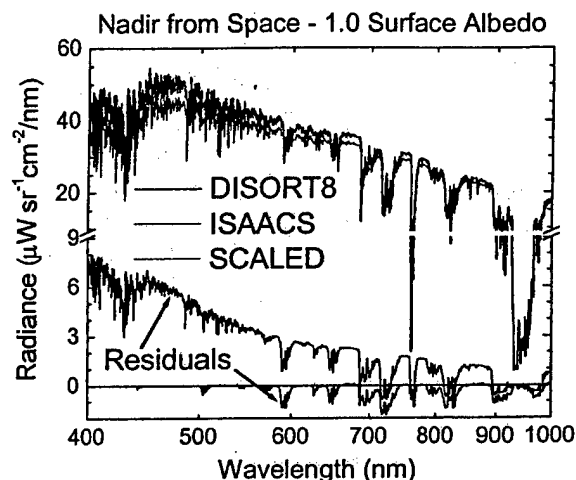


Figure 9. Results for DISORT Spectral Scaling of ISAACS Radiances with a White Surface (Albedo = 1).

## 5. CONCLUDING REMARKS AND ACKNOWLEDGEMENTS

This paper has demonstrated that MODTRAN5 provides capabilities not previously available to the research community, which are expected to add to the flexibility of atmospheric radiative transfer modeling for the community at large. The authors wish to acknowledge the generous support of the Air Force Research Laboratory (AFRL), the National Imagery and Mapping Agency (NIMA), the Spectral Information Technology Applications Center (SITAC), the Department of Energy (DOE), National Aeronautics & Space Administration (NASA). Also thanks to Dr. H.E. Snell (Atmospheric and Environmental Research, Inc.) who provided line-by-line calculations.

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